Non vanishing of high derivatives of Dirichlet L-functions at the critical point

Philippe Michel
Universite Montpellier II
34095 Montpellier cedex 5 France

Jeffrey VanderKam
Institute for Advanced Study
Princeton NJ 08540

Abstract

Using the mollification method, we show that for large q, at least $2/3 - O(k^{-2})$ of the set $\{\Lambda^{(k)}(\chi, 1/2)\}$ is non-zero, where $\Lambda(\chi, s)$ is the complete Dirichlet L-function and χ runs over all even primitive characters modulo q.

1 Introduction

Proving non-vanishing of automorphic L-functions and their derivatives at the center of the critical strip by analytical means has received considerable attention in recent years (see [1, 3, 4, 7, 8, 12]). In this paper, we consider the corresponding problem for L-functions attached to primitive Dirichlet characters of high level q. It is expected that none of these functions vanish at the point $1/2$, in fact, the low-lying zeros should be "repelled" away from that point, due to an underlying unitary symmetry (see [6]). In [4] it is shown that at least $1/3$ of these functions do not vanish at the center of the critical strip. Here we extend the non-vanishing results to arbitrary derivatives. Our approach follows that of Iwaniec-Sarnak [4] together with that of Conrey [2]. It should be pointed out that, unlike the case of automorphic L-functions, there is no known arithmetic significance to these values.

For simplicity, we consider only the case of even characters χ (that is, $\chi(-1) = 1$), odd characters may be treated in a simlilar fashion. Let $\mathcal{C}_q$ denote the set of primitive characters modulo q, and let $\mathcal{C}_q^e$ denote those which are even. Given $\chi \in \mathcal{C}_q^e$, we define

$$\Lambda(\chi, s) = \hat{q}^s \Gamma(\frac{s}{2}) L(\chi, s); \quad \hat{q} := \sqrt{\frac{q}{\pi}}.$$

This satisfies the functional equation

$$\Lambda(\chi, s) = \varepsilon_\chi \Lambda(\overline{\chi}, 1-s); \quad \varepsilon_\chi = \frac{\tau(\chi)}{q^{1/2}},$$

where $\tau(\chi)$ is the Gauss sum. From this one immediately has

$$\Lambda^{(k)}(\chi, s) = (-1)^k \varepsilon_\chi \Lambda^{(k)}(\overline{\chi}, 1-s) \tag{1}$$

for any $k \geq 1$. The main result of this paper is the following.

Theorem 1 *For any fixed $k \geq 1$ denote by p_k the limit*

$$p_k := \liminf_{q \to +\infty} \frac{|\{\chi \in \mathcal{C}_q^e : \Lambda^{(k)}(\chi, \frac{1}{2}) \neq 0\}|}{|\mathcal{C}_q^e|}.$$

Then

$$p_k \geq 2/3 - \frac{1}{36k^2} + \frac{c}{k^4},$$

where c is an absolute constant. In particular,

$$p_1 \geq 0.92 \times \frac{2}{3},\ p_2 \geq 0.98 \times \frac{2}{3},\ p_3 \geq 0.99 \times \frac{2}{3}.$$

As in [9], this is proved by comparing mollified first and second moments of the set $\{\Lambda^{(k)}(\chi, 1/2)\}$, and using Cauchy's inequality. The result is analogous to that of [2] and [9], with one exception. In both of those cases the limit for large k was the maximum possible: almost all zeros of $\xi^{(k)}$ are on the critical line and almost half of the $L_f^{(k)}(1/2)$'s are non-zero (since half are odd and half are even, this is the best possible). Here, although we expect that all of the kth derivatives are non-zero, we are only able to get to 2/3. This arises because the values of the L-functions in question come from the combination of two terms which have essentially independent arguments in the complex plane. The mollifiers we use act well on each of the terms individually, but are unable to mollify their sum in as effective a fashion. As a result, a new term arises in the calculation of the second moment, unlike any term in [9], and this prevents the proportion from exceeding 2/3.

The questions considered in this paper arose during the authors' work with Emmanuel Kowalski, and they thank him for several useful discussions on the topic. It is also a pleasure to thank B. Conrey, H. Iwaniec, P. Sarnak, and K. Soundararajan for their comments and assistance in understanding the techniques used in this paper.

2 Background

Our first step is to express the central value $\Lambda^{(k)}(\chi, 1/2)$ and its square in terms of rapidly converging series. There are several ways to achieve this goal, here we follow the presentation of [3]. Let $G(s)$ be an even polynomial with real coefficients such that $G(0)\Gamma(1/4) = 1$ and G vanishes at order at least $k+1$ at $s = -1/2,\ -5/2$. Let

$$I(\chi) := \frac{1}{2\pi i} \int_{2} \Lambda^{(k)}(\chi, s + \frac{1}{2}) G(s) \frac{ds}{s},$$

so that a contour shift and (1) give

$$\Gamma(1/4)^{-1} \Lambda^{(k)}(\chi, \frac{1}{2}) = I(\chi) + (-1)^k \varepsilon_\chi I(\overline{\chi})$$

with

$$I(\chi) := \sum_{n\geq 1} \chi(n)(\frac{\hat{q}}{n})^{1/2} V(\frac{n}{\hat{q}}),$$

$$V(y) := \frac{1}{2\pi i}\int_{(2)} \Psi(y,s)G(s)\frac{ds}{s},$$

$$\Psi(y,s) := \frac{\partial^k}{\partial^k s} y^{-s}\Gamma(\frac{s}{2}+\frac{1}{4}),$$

so that

$$\Lambda^{(k)}(\chi,\frac{1}{2}) = \Gamma(1/4)\sum_{n\geq 1}\chi(n)(\frac{\hat{q}}{n})^{1/2}V(\frac{n}{\hat{q}}) \tag{2}$$

$$+(-1)^k\varepsilon_\chi\Gamma(1/4)\sum_{n\geq 1}\overline{\chi}(n)(\frac{\hat{q}}{n})^{1/2}V(\frac{n}{\hat{q}}).$$

Similarly, since $\Lambda^{(k)}(\chi,s)\Lambda^{(k)}(\overline{\chi},s)$ is even for χ even, a contour shift gives

$$|\Lambda^{(k)}(\chi,\frac{1}{2})|^2 = 2\Gamma(1/4)^2\hat{q}\sum_{n_1}\sum_{n_2}\frac{\chi(n_1)\overline{\chi}(n_2)}{(n_1n_2)^{1/2}}W(\frac{n_1}{\hat{q}},\frac{n_2}{\hat{q}}) \tag{3}$$

with

$$W(y,y') = \frac{1}{2\pi i}\int_{(2)}\Psi(y,s)\Psi(y',s)G(s)^2\frac{ds}{s}.$$

Shifting the contours defining V and W to the right or to the left and using the vanishing of G at $s=-1/2,\ -5/2$, we infer the following:

$$V(y) = (-\log y)^k + P(-\log y) + O(y^2), \qquad V(y) \ll y^{-2}, \tag{4}$$

$$W(y,y') = (-\log y)^k(-\log y')^k + Q(-\log y, -\log y') + O((yy')^2), \tag{5}$$

$$\forall j>0 \qquad W(y,y') \ll_j (yy')^{-j}. \tag{6}$$

Here $P(X)$ and $Q(X,Y)$ are polynomials of degree $k-1$ and $2k-1$, respectively. Throughout this paper, we consider k fixed, so that (unless otherwise specified) implicit constants may depend of k.

2.1 The mollifier

We now introduce a mollifier associated with χ and k, designed to lessen the contributions of the larger values of $\Lambda^{(k)}(\chi,\frac{1}{2})$ to the first and second moment. The usual strategy in these sorts of problems is to take

$$M_k^*(\chi,\frac{1}{2}) := \sum_{m\leq M}^{*}\frac{\chi(m)x_m}{m^{1/2}},$$

where the coefficients x_m have the form

$$x_m := \mu(m) P_k(\frac{\log M/m}{\log M}) \tag{7}$$

with P_k a polynomial such that $P_k(0) = 0$, $P_k(1) = 1$. However, this choice ignores the symmetry between χ and its conjugate $\overline{\chi}$ which both appear in (2). If we used M_k^*, the proof would be virtually identical to that of [9], and we would find that $p_k > 1/2 - c/k^2$ for large k. To retrieve some of the "missing mass" (and to recover the symmetry) we introduce the "twisted" mollifier

$$M_k(\chi, \frac{1}{2}) = M_k^*(\chi, \frac{1}{2}) + (-1)^k \overline{\varepsilon}_\chi M_k^*(\overline{\chi}, \frac{1}{2}) = \sum_{m \le M}^{*} (\chi(m) + (-1)^k \overline{\varepsilon}_\chi \overline{\chi}(m)) \frac{x_m}{m^{1/2}}. \tag{8}$$

This motivation led Soundararajan to introduce similarly twisted mollifiers to deal with values of the ζ function on the critical line, and he was able to significantly improve known bounds on their moments in this fashion. We note that using the techniques of this paper (with some minor adjustments) for the case $k = 0$ and $P_0(t) = t$ gives a non-vanishing fraction of $1/2$, a slight improvement over the value found in [3].

As a simple example showing why $2/3$ may be the best result possible with the new mollifier, consider the set of numbers $e(\alpha_k) + e(\alpha_k + k/q)$, where k goes from 0 to $q-1$ (as usual, we let $e(x)$ denote $e^{2\pi i x}$). Using the mollifier $e(-\alpha_k)$, which optimally mollifies the first term, we would find a first moment of 1 and a second moment of 2, so that at least $1/2$ of the elements do not vanish. But were we to use $e(-\alpha_k) + e(-\alpha_k - k/q)$ instead, the first and second moments are 2 and 6, respectively, for a non-vanishing fraction of $2^2/6 = 2/3$. Since one expects the angles between the two terms in (2) to be uniformly distributed (this is not hard to show for the ϵ_χ's by themselves), and M_k^* does an essentially optimal job (for large k) of mollifying the first term in (2), this model may be quite accurate. It is likely, then, that finding higher non-vanishing fractions will require taking higher moments. While it is likely possible to calculate the fourth moments (this has been done for L-functions for automorphic forms, see [10]), to get the non-vanishing fraction to approach one would require arbitrarily high moments, which is far beyond current methods.

3 The mollified first moment

We wish to estimate the first moment

$$\mathcal{L}(P_k) := \sum_{\chi}^{+} \Lambda^{(k)}(\chi, \frac{1}{2}) M_k(\chi, \frac{1}{2}) \tag{9}$$

$$= \Gamma(\frac{1}{4}) \hat{q}^{1/2} \sum_{m \le M} \frac{x_m}{m^{1/2}} \sum_n \frac{1}{n^{1/2}} V(\frac{n}{\hat{q}}) \sum_{\chi}^{+} (\chi(m) + (-1)^k \overline{\varepsilon_\chi \overline{\chi}(m)})(\chi(n) + (-1)^k \varepsilon_\chi \overline{\chi}(n))$$

Since $\overline{\varepsilon}_\chi = \varepsilon_{\overline{\chi}}$, the innermost sum is

$$2 \sum_{\chi}^{+} \chi(mn) + 2(-1)^k \sum_{\chi}^{+} \varepsilon_\chi \chi(m) \overline{\chi}(n).$$

This is evaluated in [3], where it is shown that the main contribution comes from the term $mn = 1$. Using (4), (5), and (6) and following [3], we obtain for $M = \hat{q}^{\Delta}$, $\Delta < 1$,

$$\begin{aligned}\mathcal{L}(P_k) &= 2\Gamma(1/4)\phi^+(q)\hat{q}^{1/2}V(\frac{1}{\hat{q}}) + O(M^{1/2}q^{3/4}\log^k q + Mq^{1/4}\tau(q)\log^k q) \\ &= 2\phi^+(q)\hat{q}^{1/2}\log^k \hat{q}(1 + O_\Delta(\frac{1}{\log q})) \end{aligned} \quad (10)$$

where

$$\phi^+(q) = \frac{\phi^*(q)}{2}, \ \phi^*(q) = \sum_{q_1 q_2 = q} \mu(q_1)\phi(q_2) = |\mathcal{C}_q|.$$

Note that

$$|\mathcal{C}_q^e| = \phi^+(q) + O(1),$$

so the first moment, $\mathcal{L}(P_k)/|C_q^e|$, is asymptotic to $q^{1/4}\log^k q$.

4 The mollified second moment

We next estimate the mollified second moment

$$\mathcal{Q}(P_k) := \sum_{\chi}{}^{+} |\Lambda^{(k)}(\chi, \frac{1}{2})M_k(\chi, \frac{1}{2})|^2,$$

which, using $|\Lambda^{(k)}(\chi, \frac{1}{2})|^2 = |\Lambda^{(k)}(\overline{\chi}, \frac{1}{2})|^2$, splits up further into

$$\mathcal{Q}(P_k) = 2 \sum_{m_1, m_2 \le M}{}^{*} \frac{x_{m_1} x_{m_2}}{(m_1 m_2)^{1/2}} \Big(\mathcal{B}(m_1, m_2) + (-1)^k \mathcal{B}'(m_1 m_2)\Big),$$

$$\mathcal{B}(m_1, m_2) := \sum_{\chi}{}^{+} |\Lambda^{(k)}(\chi, 1/2)|^2 \chi(m_1)\overline{\chi}(m_2);$$

$$\mathcal{B}'(m) := \sum_{\chi}{}^{+} |\Lambda^{(k)}(\chi, 1/2)|^2 \varepsilon_\chi \chi(m).$$

We split $\mathcal{Q}(P_k)$ into two terms correspondingly

$$\mathcal{Q}(P_k) = 2\mathcal{Q}_1(P_k) + 2\mathcal{Q}_2(P_k). \quad (11)$$

The former matches that of [3] for $k = 0$, while the latter is a new term arising from the use of the twisted mollifier. We will evaluate $\mathcal{Q}_1(P_k)$ and $\mathcal{Q}_2(P_k)$ separately and find that both contribute asymptotically to the second moment.

5 Treatment of $\mathcal{Q}_1(P_k)$

We begin with analysis of $\mathcal{Q}_1(P_k)$. There are several ways to evaluate this (see [9] for another method), here we follow [2]. Setting $c = (m_1, m_2)$, we note that when $(m_1m_2, q) = 1$, we have $\mathcal{B}(m_1, m_2) = \mathcal{B}(m_1/c, m_2/c)$ so that

$$\mathcal{Q}_1(P_k) = \sum_{c\leq M}^{*} \sum_{\substack{m_1,m_2\leq M/c \\ (m_1,m_2)=1}}^{*} \frac{x_{cm_1}x_{cm_2}}{c(m_1m_2)^{1/2}} \mathcal{B}(m_1, m_2).$$

We have (see [3])

$$\mathcal{B}(m_1, m_2) = \Gamma(\frac{1}{4})^2 \hat{q} \sum_{q_1q_2=q} \mu(q_1)\phi(q_2) \sum_{m_1n_1\equiv\pm m_2n_2(q_2)}^{*} \frac{1}{\sqrt{n_1n_2}} W(\frac{n_1}{\hat{q}}, \frac{n_2}{\hat{q}}),$$

and after averaging over m_1, m_2 the main term will come from the (even) diagonal $m_1n_1 = m_2n_2$. Since $(m_1, m_2) = 1$ one has $n_1 = dm_2$, $n_2 = dm_1$, and the main term is

$$\mathcal{B}^{main}(m_1, m_2) = \Gamma(\frac{1}{4})^2 \hat{q}\phi^*(q) \frac{1}{(m_1m_2)^{1/2}} \sum_{d\geq 1}^{*} \frac{1}{d} W(\frac{dm_1}{\hat{q}}, \frac{dm_2}{\hat{q}}). \tag{12}$$

Using (6) we find that for $\Delta < 1$

$$\mathcal{Q}_1(P_k) = \sum_{c\leq M}^{*} \sum_{\substack{m_1,m_2\leq M/c \\ (m_1,m_2)=1}}^{*} \frac{x_{cm_1}x_{cm_2}}{c(m_1m_2)^{1/2}} \mathcal{B}^{main}(m_1, m_2) + O_\Delta(\phi^+(q)\hat{q}) \tag{13}$$

5.1 Evaluation of a series

We evaluate the innermost sum of (12) by expanding W:

$$\sum_{(d,q)=1} \frac{1}{d} W(dy, dy') = \frac{1}{2\pi i} \int_{(2)} \sum_{d\geq 1}^{*} \frac{\Psi(dy, s)\Psi(dy', s)}{d} G(s)^2 \frac{ds}{s}.$$

Expanding the Ψ's through the binomial formula, this decomposes into a linear combination over $0 \leq i + j, i' + j' \leq k$ of integrals of the form:

$$\frac{(-\log y)^i(-\log y')^{i'}}{2\pi i} \int_{(2)} \zeta_q^{(j+j')}(1 + 2s)\Gamma^{(k-i-j)}(\frac{s}{2} + \frac{1}{4})\Gamma^{(k-i'-j')}(\frac{s}{2} + \frac{1}{4}) \frac{G(s)^2}{(yy')^s} \frac{ds}{s}.$$

Shifting the contour to $\Re s = -2$ we have only the pole at $s = 0$, so this integral is

$$Res_{(i,j,i',j')} + O(\log^{2k} q(yy')^2) \tag{14}$$

where

$$Res_{(i,j,i',j')} = (-\log y)^i(-\log y')^{i'} P_{(i,j,i',j')}(-\log yy')$$

with $P_{(i,j,i',j')}$ a polynomial of degree $j+j'+1$ whose coefficients are linear combinations of

$$\omega^{(l)}(q) := \frac{d^l}{d^l s}\omega_s(q)|_{s=0},\ \omega_s(q) := \prod_{p|q}(1-\frac{1}{p^{1+2s}}).$$

In particular, when $i+j=i'+j'=k$ we find that

$$P_{(i,j,i',j')}(X) = -\frac{(-X/2)^{j+j'+1}}{j+j'+1} + \mathcal{O}(X^{j+j'}).$$

Thus the first term of (14) contributes terms of size $(\log q)^{2k+1}$ to $\mathcal{B}(m_1,m_2)$, while the second term contributes a negative power of q (since $m_1, m_2 < \hat{q}^{\Delta}$). We thus may write

$$\begin{aligned}\mathcal{B}^{main}(m_1,m_2) \;\;=\;\; & -\Gamma(\frac{1}{4})^2\hat{q}\phi^*(q)\frac{\phi(q)}{q}\frac{1}{(m_1m_2)^{1/2}}\times \\ & \Big[\sum_{j_1,j_2=0}^{k}\frac{C_k^{j_1}C_k^{j_2}}{j_1+j_2+1}\log(\frac{\hat{q}}{m_1})^{k-j_1}\log(\frac{\hat{q}}{m_2})^{k-j_2}(\frac{1}{2}\log\frac{m_1m_2}{\hat{q}^2})^{j_1+j_2+1} \\ & \qquad +R(\log(\frac{\hat{q}}{m_1}),\log(\frac{\hat{q}}{m_2}))\Big],\end{aligned}$$

with $R(X,Y)$ a polynomial in two variables of total degree at most $2k$ whose coefficients are linear combinations of the $\omega^{(l)}(q) \ll (\log\log q)^l$ for $l \le k$. In the sequel we deal only with the first part of $\mathcal{B}^{main}(m_1,m_2)$ which by abuse of notation we still call $\mathcal{B}^{main}(m_1,m_2)$. The contribution of the remaining part can be estimated in exactly the same way, since any cancellation will come from the x_{cm}'s, not the specific coefficients of $\mathcal{B}^{main}$. It will generate an error term which is at most $O(\mathcal{Q}_1(P_k)\frac{(\log\log q)^{2k}}{\log q})$.

5.2 Evaluation of a quadratic form

To evaluate $\mathcal{B}^{main}(m_1,m_2)$ exactly we start by noting the identity

$$\sum_{j_1,j_2=0}^{k}\frac{C_k^{j_1}C_k^{j_2}}{j_1+j_2+1}X^{k-j_1}Y^{k-j_2}Z^{j_1+j_2+1} = Z\int_0^1(X+tZ)^k(Y+tZ)^k dt.$$

¿From (13) and the preceding discussion we need to evaluate

$$\begin{aligned}\mathcal{Q}^m(P_k) \;\;:=\;\; & \sum_{c\le M}{}^{*}\sum_{(m_1,m_2)=1}{}^{*}\frac{x_{cm_1}x_{cm_2}}{c(m_1m_2)^{1/2}}\mathcal{B}^{main}(m_1,m_2) \\ =\;\; & \sum_{c,d}{}^{*}\frac{\mu(d)}{cd}\sum_{m_1,m_2}{}^{*}\frac{x_{cdm_1}x_{cdm_2}}{(m_1m_2)^{1/2}}\mathcal{B}^{main}(dm_1,dm_2) \\ =\;\; & \Gamma(\frac{1}{4})^2\hat{q}\frac{\phi(q)}{q}\phi^+(q)\sum_{c,d}{}^{*}\frac{\mu(d)}{cd^2}Q_{c,d}\end{aligned}$$

with

$$Q_{c,d} := \sum_{m_1,m_2}^{*} \frac{x_{cdm_1} x_{cdm_2}}{m_1 m_2} \log(\frac{\hat{q}^2}{dm_1 dm_2}) \times$$
$$\int_0^1 ((1-\frac{t}{2}) \log(\frac{\hat{q}}{dm_1}) - \frac{t}{2} \log(\frac{\hat{q}}{dm_2}))^k ((1-\frac{t}{2}) \log(\frac{\hat{q}}{dm_2}) - \frac{t}{2} \log(\frac{\hat{q}}{dm_1}))^k dt.$$

Thus we need to evaluate sums for $0 \le j \le 2k+1$ of the form

$$\sum_{cdm \le M}^{*} \frac{x_{cdm}}{m} (\log \frac{\hat{q}}{dm})^j = \mu(cd) \sum_{\substack{cdm \le M \\ (m,cd)=1}}^{*} \frac{\mu(m)}{m} (\log \frac{\hat{q}}{dm})^j P_k(\frac{\log M/cdm}{\log M}). \tag{15}$$

We now recall Lemmas 10 and 11 of Conrey [2], which will allow us to evaluate sums of this type.

Lemma 1 *Let p be a real polynomial with $p(0) = 0$; for $l \le M$, $(l,q) = 1$ let*

$$S_j(l) := \sum_{\substack{lm \le M \\ (m,lq)=1}} \frac{\mu(m)}{m} (-\log m)^j p(\frac{\log M/lm}{\log M}).$$

Then $S_j(l) = M_j(l) + O(E_j(l))$ with

$$M_0(l) = \frac{1}{\omega(lq) \log M} p'(\frac{\log M/l}{\log M}),$$

$$M_1(l) = \frac{1}{\omega(lq)} p(\frac{\log M/l}{\log M}),$$
$$M_j(l) = 0, \;\; j \ge 2,$$
$$E_j(l) = (\log M)^{j-2} (\log\log M)^4 (1 + \log M (\frac{l}{M})^b) \prod_{p|lq} (1 + \frac{1}{p^{1-2\delta}})^2,$$
$$\delta = 1/\log\log M, \;\; b \gg 1/\log\log M.$$

The trivial estimate for $S_j(l)$ is $O((\log M)^{j-1})$ (because $\zeta^{-1}(s)$ has a zero at $s = 1$), and on average we have

$$\sum_{l \le M} \frac{S_j(l) E_{j'}(l)}{l} \ll (\log M)^{j+j'-2+\epsilon},$$

so a power of *log* is saved in the error terms (we will be taking $j + j' = 2k + 1$, so the contribution to $\mathcal{Q}^m(P_k)$ of the error terms will be at most $(\log q)^{2k-1+\epsilon}$, which we can ignore).

Lemma 2 *Let $f(p) = 1 + O(p^{-c})$ for $c > 0$. Put $f(r) := \prod_{p|r} f(p)$, and*

$$J_j(M) = \sum_{l \le M} \frac{\mu^2(l)}{l} f(l)(\log \frac{M}{l})^j$$

for $j \ge 0$ an integer. Then

$$J_j(M) = \Big(\prod_p (1 + \frac{f(p)}{p})(1 - \frac{1}{p})\Big) \frac{\log^{j+1} M}{j+1} + O((\log M)^j).$$

Returning to (15), we expand

$$(\log \frac{\hat{q}}{dm})^j = (\log \frac{\hat{q}}{d})^j - j(\log \frac{\hat{q}}{d})^{j-1} \log m + \dots.$$

By Lemma 1 and averaging over cd, only these two first terms give a significant contribution, so the sum (15) equals

$$\frac{\mu(cd)}{\omega(qcd)}[\frac{(\log \hat{q}/d)^j}{\log M} P_k'(\frac{\log M/cd}{\log M}) + j(\log \hat{q}/d)^{j-1} P_k(\frac{\log M/cd}{\log M}) + O(\log q^{j-2} E_2(cd))].$$

Thus for $\mu^2(cd) = 1, (cd, q) = 1$ the main term of $Q_{c,d}$ is (set $u = \frac{\log M/cd}{\log M}$ to save space)

$$\begin{aligned}
Q^m_{c,d} &= 2(\frac{\mu(cd)}{\omega(qcd)})^2 \int_0^1 \sum_{j,j'} C_k^j C_k^{j'} (1 - \frac{t}{2})^{j+k-j'} (-\frac{t}{2})^{j'+k-j} \times \\
&\quad [\frac{(\log \hat{q}/d)^{j+j'+1}}{\log M} P_k'(u) + (j + j' + 1)(\log \hat{q}/d)^{j+j'} P_k(u)] \\
&\quad [\frac{(\log \hat{q}/d)^{2k-j-j'}}{\log M} P_k'(u) + (2k - j - j')(\log \hat{q}/d)^{2k-j-j'-1} P_k(u)] \\
&:= 2(\frac{\mu(cd)}{\omega(qcd)})^2 [\frac{(\log \hat{q}/d)^{2k+1}}{(\log M)^2} P_k'(u)^2 I_1 + \frac{(\log \hat{q}/d)^{2k}}{\log M} P_k(u) P_k'(u) I_2 + \\
&\quad + (\log \hat{q}/d)^{2k-1} P_k^2(u) I_3]
\end{aligned}$$

with

$$I_1 := \int_0^1 \sum_{j,j'} C_k^j C_k^{j'} (1 - \frac{t}{2})^{j+k-j'} (-\frac{t}{2})^{j'+k-j} dt = \frac{1}{2k+1},$$

$$I_2 := \int_0^1 \sum_{j,j'} C_k^j C_k^{j'} (1 - \frac{t}{2})^{j+k-j'} (-\frac{t}{2})^{j'+k-j} (1 + j + j' + 2k - (j + j'))dt = (2k+1) I_1 = 1,$$

$$I_3 := \int_0^1 \sum_{j,j'} C_k^j C_k^{j'} (1 - \frac{t}{2})^{j+k-j'} (-\frac{t}{2})^{j'+k-j} (1 + j + j')(2k - (j + j'))dt.$$

To compute the last integral we use the identities

$$(1 + j + j')(2k - (j + j')) = (k - j) + (k - j') + j(k - j) + j'(k - j') + j(k - j') + j'(k - j),$$

$$(X+Y)^k = \sum_j C_k^j X^j Y^{k-j},$$

$$kX(X+Y)^{k-1} = \sum_j C_k^j j X^j Y^{k-j},$$

$$k(k-1)XY(X+Y)^{k-2} = \sum_j C_k^j j(k-j) X^j Y^{k-j},$$

to find that

$$I_3 = kI_1 - \frac{(k-1)k}{(2k-1)(2k+1)} + \frac{2k^3}{(2k-1)(2k+1)} = \frac{k^2}{2k-1}. \tag{16}$$

We thus have

$$\mathcal{Q}_1(P_k) \simeq 2\Gamma(\frac{1}{4})^2 \hat{q}\phi^+(q)\omega^{-1}(q) \sum_{c,d}{}^{*} \frac{\mu^2(cd)\mu(d)}{cd^2\omega(cd)^2} (\log \hat{q}/d)^{2k-1}$$

$$\times[\frac{(\log \hat{q}/d)^2}{(\log M)^2}\frac{P_k'(u)^2}{2k+1} + \frac{(\log \hat{q}/d)}{\log M} P_k(u)P_k'(u) + \frac{k^2 P_k^2(u)}{2k-1}].$$

In the bracket, we can forget the term d in the $\log(\hat{q}/d)$ since the terms in $\log d$ will yield smaller powers of $\log \hat{q}$. So we evaluate for a given polynomial P

$$S_P := \sum_{m\le M}{}^{*} \frac{\mu^2(m)}{m\omega^2(m)} \frac{\phi(m)}{m} P_k(\frac{\log M/m}{\log M})$$

By Lemma 2, this is

$$S_P = \omega(q)(\log M + O(1)) \int_0^1 P_k(t)dt$$

so that

$$\frac{\mathcal{Q}_1(P_k)}{(\log \hat{q})^{2k}} = 2\Gamma(\frac{1}{4})^2 \hat{q}\phi^+(q)(1+O(\frac{\log_2^{2k} q}{\log q}))\left[\frac{1}{\Delta}\int_0^1 \frac{P_k'(t)^2}{2k+1}dt + \frac{1}{2} + \Delta \int_0^1 \frac{k^2 P_k(t)^2}{2k-1}dt\right]. \tag{17}$$

6 Treatment of $\mathcal{Q}_2(P_k)$

We now evaluate $\mathcal{Q}_2(P_k)$. ¿From (3), we recall the identity (see [3]) for $(m,q)=1$

$$\sum_{\chi}{}^{+} \varepsilon_\chi \chi(m) = \frac{1}{q^{1/2}} \sum_{\substack{q_1q_2=q\\(q_1,q_2)=1}} \mu^2(q_1)\phi(q_2)\cos(2\pi\frac{\overline{mq_1}}{q_2}) \tag{18}$$

and obtain

$$\mathcal{B}'(m) = 2\Gamma(\frac{1}{4})^2 \frac{\hat{q}}{q^{1/2}} \sum_{q_1q_2=q} \mu(q_1)\phi(q_2) \sum_{n_1,n_2}{}^{*} \cos(2\pi n_2 \frac{\overline{q_1mn_1}}{q_2})(n_1n_2)^{-1/2} W(\frac{n_1}{\hat{q}}, \frac{n_2}{\hat{q}}). \tag{19}$$

We start by evaluating the sum over n_2.

Lemma 3 *Given $q = q_1q_2$, with $(q_1, q_2) = 1$, a with $(a, q_2) = 1$, and f with Mellin transform $\hat{f}(s)$ defined and rapidly decaying on vertical strips on $\Re s > 1/2$,*

$$\sum_{\substack{(n,q_1q_2)=1\\ \cos}} (2\pi \frac{n\bar{a}}{q_2}) f(n) = \frac{\phi(q_1)}{q_1} \frac{\mu(q_2)}{q_2} \hat{f}(1)$$

$$+ \sum_{r_1|q_1} \frac{\mu(r_1)}{r_1} \sum_{r_2|q_2} \frac{\mu(r_2)}{r_2} \sum_{na\equiv\pm r_1(q_2/r_2)} \frac{1}{2\pi i} \int_{(1/3)} \hat{f}(1-s)\Gamma(s) \sin\frac{\pi}{2}s \left(\frac{q_2r_1}{2\pi n}\right)^s ds.$$

This comes from Poisson summation, or, equivalently, through the functional equation of the Hurwitz zeta function (see [5] for the method used in a more difficult setting). One starts by modifying f so that it vanishes at the origin, but an approximation argument then allows one to take all f whose Mellin transforms are defined along the contour in question.

We thus have

$$B'(m) = \frac{2\Gamma(1/4)^2}{\sqrt{\pi}} \frac{\mu(q)\phi(q)}{q} \sum_{\substack{q_1q_2=q\\ (q_1,q_2)=1}} \sum_{(n_1,q)=1} n_1^{-1/2} \int_0^\infty W(\frac{n_1}{\hat{q}}, \frac{x}{\hat{q}}) \frac{dx}{x^{1/2}} \tag{20}$$

$$+ \frac{2\Gamma(1/4)^2}{\sqrt{\pi}} \sum_{\substack{q_1r_1q_2r_2=q\\ (q_1r_1,q_2r)=1}} \mu(q_1r_1)\phi(q_2r_2) \frac{\mu(r_1)}{r_1} \frac{\mu(r_2)}{r_2}$$

$$\sideset{}{^*}\sum_{n_1n_2mq_1\equiv\pm1(q_2)} n_1^{-1/2} \frac{1}{2\pi i} \int_{(1/3)} (\frac{q_2r_1r_2}{2\pi n_2})^s \Gamma(s) \sin\frac{\pi}{2}s \int_0^\infty W(\frac{n_1}{\hat{q}}, \frac{x}{\hat{q}}) \frac{dx}{x^{1/2+s}} ds.$$

By the definition of the Mellin transform,

$$\int_0^\infty W(\frac{n_1}{\hat{q}}, \frac{x}{\hat{q}}) \frac{dx}{x^\alpha} = \sum_{j=0}^{k} (-1)^j \binom{k}{j} \partial_t^j \left[\frac{G(t)^2}{t} \partial_t^k (\frac{\hat{q}^t}{n_1^t} \Gamma(\frac{t}{2} + \frac{1}{4})) \partial_t^{k-j} (\hat{q}^t \Gamma(\frac{t}{2} + \frac{1}{4})) \right]_{t=1-\alpha} \tag{21}$$

so long as $\alpha < 1$. We will return to this expression in detail later, for now it is enough to note that it is holomorphic on $\alpha < 3/2$, decays rapidly in vertical strips, and is dominated by

$$\hat{q}^{2-2\alpha+\epsilon} n_1^{\alpha-1}$$

for any $\epsilon > 0$.

We now look to bound

$$\sum_{m_1,m_2} \frac{x_{m_1}x_{m_2}}{(m_1m_2)^{1/2}} B'(m_1m_2).$$

The first term of (20) is easier, so we do it first. Since the x_m's are bounded, the contribution of the first term of (20) is dominated by

$$\hat{q}^{1+\epsilon} \sum_{m_1,m_2} \frac{1}{(m_1m_2)^{1/2}} \sum_{n_1} \frac{1}{n_1}.$$

Since we can ignore those n_1 terms which are larger than $\hat{q}^{1+\epsilon}$, this is at most

$$\hat{q}^{1+\epsilon}M,$$

which is smaller than $q^{3/2}$ so long as $\Delta < 2$.

We thus turn to the second term of (20). The first thing to consider is what bounds there may be on n_2 (note that this is the dual variable to the original n_2, so we do not necessarily have the $n_2 << \hat{q}^{1+\epsilon}$ bound). Expanding (21), we are interested in a finite sum of various factors of $\log \hat{q}$ and $\log n_1$ times integrals of the form

$$\int_{(1/3)} \left(\frac{q_2 r_1 r_2 n_1}{2\pi n_2 \hat{q}^2}\right)^s F(s)ds,$$

where $F(s)$ is holomorphic on the right half-plane, has exponential decay in vertical strips, and grows roughly as $\Gamma(s)$ as s moves to the right along the real axis. Note also that the expression in parentheses is actually just $n_1/(2n_2q_1)$. From a contour shift to the left, we can bound the integral by

$$c_A \left(\frac{n_2 q_1}{n_1}\right)^{-A}.$$

Thus the contribution from $n_2 > n_1\hat{q}^\delta$ is dominated by any negative power of q, so we can assume that $n_2 < n_1 q^\delta << \hat{q}^{1+\delta}$.

Returning to the second term of (20) and shifting the s contour close to zero, the contribution is bounded by

$$\sum_{\substack{q_1r_1q_2r_2=q \\ (q_1r_1,q_2r_2)=1}} \phi(q_2r_2)(r_1r_2)^{-1}(q_2r_1r_2)^{1/2} \sum_{m_1m_2n_1n_2q_1\equiv\pm1(q_2)} \frac{1}{(m_1m_2n_1n_2)^{1/2}}. \tag{22}$$

Suppose first that $m_1m_2n_1n_2 > q_2$. There are two possible values for this product in each range of q_2, and the product is at most $\hat{q}^{2+2\Delta+\delta}$, so (22) is dominated by

$$q^\epsilon \sum_{\substack{q_1r_1q_2r_2=q \\ (q_1r_1,q_2r_2)=1}} \phi(q_2r_2)\frac{1}{(r_1r_2)^{1/2}} \sum_{k<\hat{q}^{2+2\Delta+\delta}/q_2} \frac{1}{k^{1/2}} << \hat{q}^{1+\Delta+\delta/2+\epsilon} \sum_{q_2r_2|q} \frac{\phi(q_2r_2)}{(q_2r_2)^{1/2}} << q^{1+\Delta/2+\delta/4+\epsilon}.$$

The choice of δ was arbitrary, so as long as $\Delta < 1$, this is smaller than the main term.

Now suppose that $m_1m_2n_1n_2 < q_2$. The sum is then dominated by

$$\sum_{\substack{q_1r_1q_2r=q \\ (q_1r_1,q_2r_2)=1}} \phi(q_2r_2)\frac{q_2^{1/2}}{(r_1r_2)^{1/2}} \left(\frac{1}{\overline{q_1}^{1/2}} + \frac{1}{\overline{-q_1}^{1/2}}\right), \tag{23}$$

where $\overline{a}$ denotes the inverse of a modulo q_2. If $q_1 \neq 1$, then $q_1\overline{q_1} > q_2$, while for any value of q_1 we have $q_1\overline{-q_1} \geq q_2 - 1 >> q_2$ (if q_2 is close to one, then (23) is trivially smaller than $q^{3/2}$). Thus, so long as $q_1 \neq 1$, (23) is bounded by

$$\sum_{q_1r_1q_2r_2=q} \phi(q_2r_2)\frac{q_1^{1/2}}{(r_1r_2)^{1/2}} << q^{1+\epsilon},$$

which is easily small enough to ignore.

Thus we are left with the case $q_1 = 1$, $m_1m_2n_1n_2q_1 \equiv 1(q_2)$, $m_1m_2n_1n_2 < q_2$, which is to say, $m_1 = m_2 = n_1 = n_2 = q_1 = 1$. This particular case will contribute a main term to the second moment, coming entirely from the angles of the ϵ_χ's, and (essentially) not at all from the quality of the mollifier. This term is now

$$\frac{2\Gamma(1/4)^2}{\sqrt{\pi}} \sum_{\substack{r_1q_2r_2=q \\ (r_1,q_2r_2)=1}} \mu(r_1)\phi(q_2r_2)\frac{\mu(r_1r_2)}{r_1r_2}\frac{1}{2\pi i}\int_{(1/3)}\left(\frac{q}{2\pi}\right)^s \Gamma(s)\sin\frac{\pi}{2}s$$

$$\sum_{j=0}^{k}(-1)^j\binom{k}{j}\partial_t^j\left[\frac{G(t)^2}{t}\partial_t^k(\hat{q}^t\Gamma(\frac{t}{2}+\frac{1}{4}))\partial_t^{k-j}(\hat{q}^t\Gamma(\frac{t}{2}+\frac{1}{4}))\right]_{t=1/2-s} ds.$$

All we are interested in is the main term as $q \to \infty$, so we only differentiate the $\hat{q}^t$ terms in the parentheses of the second line. Changing s to $1/2 - t$ throughout the integral, we get

$$\frac{2\Gamma(1/4)^2}{\sqrt{\pi}} \sum_{\substack{r_1q_2r_2=q \\ (r_1,q_2r_2)=1}} \mu(r_1)\phi(q_2r_2)\frac{\mu(r_1r_2)}{r_1r_2}\frac{1}{2\pi i}\int_{(1/6)}\left(\frac{q}{2\pi}\right)^{(1/2-t)} \Gamma(\frac{1}{2}-t)\sin(\frac{\pi}{4}-\frac{\pi}{2}t)$$

$$G(t)^2\Gamma(\frac{1}{4}+\frac{t}{2})^2\sum_{j=0}^{k}(-1)^j\binom{k}{j}(\log\hat{q})^{2k-j}\partial_t^j\left[\hat{q}^{2t}t^{-1}\right] dt.$$

Since $(q/2\pi)^{1/2-t}\hat{q}^{2t} = \hat{q}^{1/2}2^{t-1/2}$, this integrand does not depend on q^t, so that any differentiation of t^{-1} will contribute lower orders in $\log\hat{q}$. Thus the sum on j is just $t^{-1}(-1)^k(\log\hat{q})^{2k}$, and the sum on r_1, r_2, q_2 (which completely separates from the integral) is

$$\sum_{\substack{r_1q_2r_2=q \\ (r_1,q_2r_2)=1}} \mu(r_1)\phi(q_2r_2)\frac{\mu(r_1r_2)}{r_1r_2} = \phi^*(q),$$

so the main term of $\mathcal{B}'(1)$ is

$$(-1)^k\frac{2\Gamma(1/4)^2}{\sqrt{\pi}}\phi^*(q)\hat{q}(\log\hat{q})^{2k}\frac{1}{2\pi i}\int_{(1/6)} 2^{t-1/2}\Gamma(\frac{1}{2}-t)\sin(\frac{\pi}{4}-\frac{\pi}{2}t)G(t)^2\Gamma(\frac{1}{4}+\frac{t}{2})^2\frac{dt}{t}. \quad (24)$$

It thus remains to evaluate the integral. The various functional equations for Γ imply that

$$2^t\Gamma(\frac{1}{2}-t)\Gamma(\frac{1}{4}+\frac{t}{2}) = \frac{\pi}{\sin(\frac{\pi}{4}+\frac{\pi}{2}t)}\frac{\Gamma(\frac{1}{4}-\frac{t}{2})}{\sqrt{2\pi}}.$$

We also have the trigonometric identity

$$\frac{\sin(\frac{\pi}{4}-\frac{\pi}{2}t)}{\sin(\frac{\pi}{4}+\frac{\pi}{2}t)} = \frac{1-\sin\pi t}{\cos\pi t},$$

so the integral in (24) equals

$$\frac{\sqrt{\pi}}{2}\frac{1}{2\pi i}\int_{(1/6)}\Gamma(\frac{1}{4}+\frac{t}{2})\Gamma(\frac{1}{4}-\frac{t}{2})\frac{1-\sin\pi t}{\cos\pi t}G(t)^2\frac{dt}{t}.$$

The integrand is thus even or odd in t, depending on whether one takes 1 or $\sin\pi t$. Its value is then 1/2 times the residue coming from 1 at $t=0$, since it has no other poles between $\Re t = 1/6$ and $\Re t = -1/6$. We thus find that, so long as $\Delta < 1$,

$$\mathcal{Q}_2 = 2(-1)^k\mathcal{B}'(1) = 2\Gamma(\frac{1}{4})^2\phi^+(q)\hat{q}(\log\hat{q})^{2k}(1+O(\frac{1}{\log\hat{q}})). \tag{25}$$

7 Conclusion

¿From (11), (10), (17), and (25), along with Cauchy's inequality, we have

$$\begin{aligned}&\liminf_{q\to\infty}\frac{1}{\phi^+(q)}|\{\chi\in\mathcal{C}_q^e : \Lambda^{(k)}(\chi,\frac{1}{2})\neq 0\}|\\ &\geq \liminf_{q\to\infty}\frac{\left(\frac{1}{\phi^+(q)}\sum^+ M_k(\chi,\frac{1}{2})\Lambda^{(k)}(\chi,\frac{1}{2})\right)^2}{\frac{1}{\phi^+(q)}\sum^+|M_k(\chi,\frac{1}{2})\Lambda^{(k)}(\chi,\frac{1}{2})|^2}\\ &= 1/[\frac{\Delta^{-1}}{2k+1}\int_0^1 P_k'^2(t)dt + 1 + \frac{\Delta k^2}{2k-1}\int_0^1 P_k^2(t)dt].\end{aligned}$$

It thus remains to find a polynomial P_k satisfying $P_k(0) = 1 - P_k(1) = 0$ to maximize this last expression. By an approximation argument, we may replace P_k by any infinitely differentiable function with rapidly convergent Taylor series on $[0,1]$.

Equivalently, we need to minimize the functional $p \to F(p)$, where p ranges over all such Taylor series with $p(0) = 1 - p(1) = 0$ and

$$F(p) := \frac{\Delta^{-1}}{2k+1}\int_0^1 p'^2(t)dt + \frac{\Delta k^2}{2k-1}\int_0^1 p^2(t)dt.$$

As in [2], the optimal choice for $k > 0$ is

$$P_k(t) := \frac{\sinh(\Lambda t)}{\sinh(\Lambda)};\quad \Lambda = \Delta k\sqrt{\frac{2k+1}{2k-1}}.$$

A straightforward calculation then shows that

$$F(P_k) = \frac{\Delta^{-1}}{2k+1}\Lambda\coth\Lambda = \frac{k}{\sqrt{4k^2-1}}\coth\Lambda.$$

Using $p_k \geq 1/(1+F(P_k))$ and $\Delta = 1-\epsilon$ for small k then gives the values listed in the Theorem. For large k we may approximate $\coth\Lambda$ by 1, so that $F(P_k) = 1/2 + k^{-2}/16 + O(k^{-4})$, and this gives the asymptotics for p_k. Note that the asymptotic behavior of p_k is independent of the choice of Δ, except for an exponentially small term. This phenomenon also arises with automorphic L-functions (see [9]), and reflects the fact that high derivatives fluctuate less in relative size and thus require less mollification. Thus no improved bounds on the remainder terms will improve the 2/3 limit for the p_k's.

References

[1] R. Balasubramanian and V.K. Murty, Zeros of Dirichlet L functions, *Ann. Sci. Ec. Norm. Sup.* **25** (1992), 567-615.

[2] B. Conrey, Zeros of derivatives of Riemann's ξ-function on the critical line, *J. Number Theory* **16** (1983), 49-74.

[3] H. Iwaniec and P. Sarnak, Dirichlet L-functions at the central point, to appear in proceedings of the conference in honor of the 60th birthday of A. Schinzel.

[4] H. Iwaniec and P. Sarnak, non vanishing of central values of automorphic L-functions and Siegel's zeros, in preparation.

[5] M. Jutila, A method in the theory of exponential sums, Tata Lect. Notes Math. **80** (1987).

[6] N. Katz and P. Sarnak, Zeros of zeta functions and symmetry, *Bull. Amer. Math. Soc. (NS)* **36** (1999), 1-26.

[7] E. Kowalski and P. Michel, Sur les zeros de fonctions L de formes automorphes, Preprint 1997.

[8] E. Kowalski and P. Michel, A lower bound for the rank of $J_0(q)$, Preprint 1997.

[9] E. Kowalski, P. Michel and J. VanderKam, Non-vanishing of high derivatives of automorphic L-functions at the center of the critical strip, Preprint 1999.

[10] E. Kowalski, P. Michel and J. VanderKam, Mollification of the fourth moment of automorphic L-functions and arithmetic applications, in preparation.

[11] K. Soundararajan, Mean values of the Riemann zeta-function, *Mathematika* **42** (1995), 158-174.

[12] J. VanderKam, The rank of quotients of $J_0(N)$, *Duke Math. J.* (to appear).